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Predictive modeling of PFAS behavior and degradation in novel treatment scenarios: A review

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ABSTRACT

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants that resist conventional water treatment methods, raising concerns about their impact on human health and ecosystems. As PFAS contamination becomes increasingly widespread, the need for novel, effective treatment solutions have grown. Predictive modeling offers a promising approach to evaluate PFAS behavior, removal efficiency, and transformation pathways in emerging treatment technologies. This narrative review explores current advancements in predictive models for PFAS remediation, focusing on methods that incorporate PFAS structural characteristics, environmental factors, and treatment type. Three main modeling approaches are discussed: empirical, mechanistic, and machine learning models, each with unique strengths and limitations depending on data availability and treatment conditions. The review also addresses recent developments in advanced treatment systems such as advanced oxidation processes (AOPs), electrochemical treatment, and adsorption, as well as the role of machine learning in optimizing treatment predictions. Key challenges, including data limitations, transformation product toxicity, and model validation, are examined, with recommendations for future research emphasizing data expansion, integration of toxicity predictions, and enhanced model interpretability. By tailoring predictive models to PFAS-specific variables and diverse treatment conditions, researchers can advance sustainable PFAS management practices and guide effective remediation strategies for contaminated sites.

1. Introduction

Per- and polyfluoroalkyl substances (PFAS) encompass a broad group of synthetic chemicals that have been integral to various industrial applications, largely due to their unique chemical properties (Glüge et al., 2020; Brase et al., 2021; Gaines, 2023). Known for their exceptional thermal stability (Joudan and Lundgren, 2022) with a decomposition temperature ranging from 150 to 200°C (Sasi et al., 2021), water and oil repellency (Meng et al., 2023), and resistance to biological and chemical degradation (Wackett, 2022), PFAS compounds have found widespread use in products ranging from nonstick cookware and water-resistant fabrics to firefighting foams and industrial cleaning agents (Zornes et al., 2022). However, these same chemical characteristics, which make PFAS invaluable in industrial and consumer products, have also rendered them some of the most persistent contaminants in the environment (Panieri et al., 2022). This persistence stems from the strong carbon-fluorine bonds in PFAS structures, which resist breakdown by traditional environmental and biological processes (Grgas et al., 2023). As a prominent member of PFAS, perfluorooctane sulfonate (PFOS) has an octafluorinated carbon chain (C_8F_{17}) linked to a sulfonate group ($-SO_3-$) at one terminus (See Fig. 1). This configuration exhibits significant hydrophobicity owing to the fluorine atoms around the carbon chain, rendering PFOS impervious to water and oil. The sulfonate group confers a significant negative charge, enhancing its solubility in water

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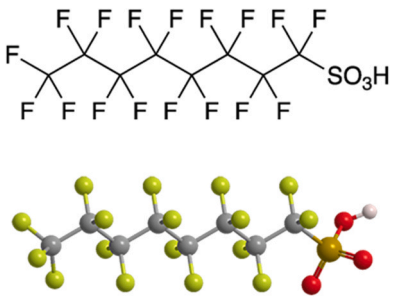

Fig. 1. Schematic representation of carbon-fluorine bonds.

and environmental persistence. The distinctive structure of PFOS renders it resistant to degradation in natural environments, resulting in extensive contamination and related health hazards. Consequently, PFAS can persist in the environment for decades, leading to widespread and pervasive contamination of water, soil, and air (Kibbey et al., 2020).

Over time, PFAS accumulation in various ecosystems has raised significant health concerns (Gagliano et al., 2020). Many PFAS compounds are bioaccumulative, meaning they build up in the tissues of living organisms, traveling through the food chain and ultimately impacting human health (Brennan et al., 2021). Numerous studies have documented potential adverse effects of PFAS exposure, including liver damage (Costello et al., 2022), immune system disruption (Beans, 2021), developmental issues (Yao et al., 2023), and increased cancer risk (Seyyedsalehi and Boffetta, 2023). PFAS exposure pathways primarily involve ingestion of contaminated drinking water, but other routes, such as food consumption, inhalation, and dermal contact, are also of concern (Domingo and Nadal, 2019). As a result, PFAS contamination has become an urgent environmental and public health issue, driving regulatory bodies, researchers, and industry stakeholders to seek effective treatment solutions.

However, the environmental resilience of PFAS poses significant challenges for conventional water treatment technologies (Wanninayake, 2021), many of which are ineffective in breaking down or removing PFAS. Processes such as coagulation, sedimentation, and biological treatment, commonly employed in wastewater treatment plants, do little to degrade PFAS compounds (Lenka et al., 2021). Advanced treatment methods, including electrochemical, sonochemical, plasma and hybrid techniques, activated carbon adsorption, ion-exchange resins, and high-energy processes like advanced oxidation, have demonstrated some effectiveness, yet these technologies often face limitations in terms of efficiency, cost, or potential by-product formation (Wanninayake, 2021). These challenges underscore the need for novel and efficient treatment approaches specifically designed to target the unique characteristics of PFAS.

Given the limitations of existing treatment methods, predictive modeling has emerged as a promising approach to improve PFAS remediation strategies (Sima and Jaffé, 2021). Predictive modeling involves the use of computational tools and algorithms to simulate the behavior, fate, and transformation of PFAS compounds in various treatment scenarios (Le et al., 2021). These models can incorporate numerous variables, including PFAS chemical structure, environmental conditions, and specific treatment methods, to predict how PFAS compounds will behave in different settings and in identifying the source of PFAS contamination in environmental samples (Kibbey et al., 2020). This approach offers several advantages: it allows researchers to experiment with different treatment methods in a virtual environment, optimizing conditions for maximum PFAS removal before physical implementation (Raza et al., 2019). For instance, recent advances in PFAS modeling in soil-water environments show promise for understanding their fate, transport, and response to remediation techniques (Sima and Jaffé, 2021). By simulating PFAS removal in diverse treatment systems, predictive models can help identify optimal treatment combinations tailored to specific PFAS profiles and environmental conditions, potentially overcoming some of the limitations seen with traditional treatment processes.

Furthermore, predictive modeling is invaluable in its capacity to anticipate the transformation and degradation pathways of PFAS compounds. Certain treatment methods, particularly those that involve high-energy processes or chemical reactions such as electrochemical oxidation, advanced reduction processes (ARPs), and plasma-based technology, has shown potential to effectively degrade PFAS compounds rather than fully mineralizing them (Nzeribe et al., 2019; Cui et al., 2020; Chen et al., 2023). This degradation can produce transformation products, some of which may retain toxicity or environmental persistence. Accurate predictive models can help in understanding these transformation products' behavior, providing essential insights into potential risks associated with partial PFAS degradation.

In recent years, advances in computational power and machine learning have further enhanced the potential of predictive modeling for PFAS treatment applications. Machine learning algorithms, for example, Random Forest, Least Absolute Shrinkage, and Feed-forward Neural Networks, can predict extremely accurate carbon-fluorine bond dissociation energies for PFAS, aiding in their efficient treatment removal by identifying patterns and correlations that might elude traditional modeling approaches (Raza et al., 2019). These data-driven models can account for complex interactions between PFAS compounds and treatment media, offering nuanced predictions of treatment efficacy. Such approaches are particularly beneficial for simulating novel treatment technologies that lack extensive field data, providing a cost-effective means of assessing their potential effectiveness and limitations. However, despite the promise of predictive modeling, significant challenges remain, particularly concerning sufficient data for training, time and cost constraints, ethical considerations, and model validation (Polyzotis et al., 2018; Wörmann et al., 2022; Shankar et al., 2023).

Ultimately, the goal of predictive modeling in PFAS treatment is to provide a science-backed foundation for developing and implementing customized remediation strategies. By offering a detailed understanding of PFAS behavior in response to different treatment types and environmental variables, predictive models can guide decision-making in both research and regulatory contexts, but they need to adhere to rigorous scientific method and adopt best modeling practice to ensure reliability (Özkundakci et al., 2018). This approach aligns with the broader trend toward sustainable environmental management, where tailored, data-driven strategies are increasingly valued over one-size-fits-all solutions. The rationale for this narrative review lies in the urgent need to understand and optimize treatment methods for PFAS, a class of highly persistent and toxic compounds. Given the limitations of conventional water treatment technologies in effectively removing or degrading PFAS, there is a pressing demand for novel, efficient, and sustainable treatment solutions. Predictive modeling offers a promising avenue to simulate PFAS behavior across different treatment scenarios, tailoring approaches based on PFAS chemical structure, environmental conditions, and the specific treatment method. This review aims to synthesize recent advancements in predictive modeling applied to PFAS removal and degradation, highlighting the approaches, challenges, and emerging technologies that can improve treatment outcomes. By compiling and analyzing current research, this review provides a comprehensive overview of predictive models in PFAS treatment, aiming to guide future studies and assist stakeholders in designing targeted and effective remediation strategies for PFAS-contaminated environments.

Table 1 presents the physical and chemical properties of PFOS, a perfluorinated molecule frequently encountered in environmental research. The empirical formula of PFOS is $C_8HF_{17}O_3S$, signifying its intricate structure comprising a perfluorinated alkyl chain and a sulfonate moiety. The substance possesses a molar mass of 500.13 g/mol and is characterised by its white powder form. The melting point of PFOS is between 258 and 260 °C, indicating its considerable stability at high temperatures, while its boiling point is not provided. PFOS exhibits

Table 1
Physico-chemical properties of PFAS.

Property	Details
Empirical formula	$C_8HF_{17}O_3S$
Molar mass	500.13 g/mol
Appearance	White powder
Boiling Point	Not available
Melting Point	258–260 °C
Water solubility	680 mg/L

Source: American Society of Nigeria

moderate solubility in water, quantified at 680 mg/L, facilitating its persistence in aquatic habitats and accumulation within ecosystems.

2. PFAS properties and challenges in treatment

The structural diversity of PFAS compounds further complicates treatment, as each variant can behave differently in terms of mobility, bioaccumulation, and reactivity under various treatment scenarios. However, characterizing the structural diversity of PFAS alternatives is important for understanding their environmental distribution, bioaccumulation, transfer, and ecological impacts (Ruan et al., 2022). This section discusses the specific properties that render PFAS challenging to treat and how these characteristics impact predictive modeling and treatment efficiency.

2.1. Chemical structure and stability

The core characteristic of PFAS compounds is the presence of carbon-fluorine bonds, which are among the strongest in organic chemistry (Langer et al., 2019). This bond strength imparts thermal and chemical stability (Joudan and Lundgren, 2022), allowing PFAS to withstand conditions that would typically degrade other organic pollutants. Structurally, PFAS can be divided into two main categories: perfluoroalkyl and polyfluoroalkyl substances (Domingo and Nadal, 2019). Perfluoroalkyl compounds, like perfluorooctanoic acid (PFOA) and PFOS, have carbon chains fully fluorinated, while polyfluoroalkyl substances contain both fluorinated and non-fluorinated carbon atoms. The length of the carbon chain in PFAS also influences their environmental behavior and toxicity, with long-chain PFAS being more bioaccumulative and often more challenging to remove compared to short-chain variants (Feng et al., 2023). Recent studies underscore that the variation in PFAS structure affects both their environmental transport and interaction with treatment media, necessitating treatment methods specifically tailored to PFAS chain length and functional groups.

2.2. Influence of functional groups on reactivity

In addition to carbon chain length, the presence of functional groups in PFAS compounds and their and hydrophilicity/hydrophobicity significantly impacts their reactivity and behavior in treatment systems (Rahman et al., 2014). For example, PFAS compounds with sulfonate groups (e.g., PFOS) differ in water solubility and treatment susceptibility compared to those with carboxylate groups (e.g., PFOA). For instance, electrochemical treatment shows potential for decomposition of PFOA and PFOS in AFFF-impacted groundwater, with 58 % and 98 % recovery as fluoride, with shorter chain PFAAs being more recalcitrant (Schaefer et al., 2015). Functional groups, surface chemistry, binding sites, and pH can influence the adsorption potential of PFAS on treatment media, such as activated carbon or ion-exchange resins, as well as their susceptibility to oxidative degradation in processes like advanced oxidation (Wu et al., 2020). Studies have shown that specific functional groups can alter how PFAS interact with reactive species generated in treatment systems, such as hydroxyl radicals in oxidation processes or reactive intermediates in electrochemical treatments. Therefore, understanding and accounting for these functional group influences is essential when designing predictive models that accurately reflect PFAS behavior under various treatment conditions.

2.3. Environmental variables affecting treatment efficiency

Environmental factors such as pH, temperature, and the presence of co-contaminants further complicate PFAS treatment (Schaefer et al., 2015). pH levels, for example, can alter the charge and solubility of PFAS compounds, affecting their interaction with treatment media. A study showed that acidic conditions can enhance PFAS adsorption on activated carbon due to the surface charge of the PAC and the properties of protonation of the PFASs, while alkaline conditions may reduce adsorption efficiency (Son et al., 2020). Temperature is another crucial variable; increased temperatures can accelerate reaction kinetics in oxidative and electrochemical processes (Alam et al., 2020), potentially improving PFAS degradation rates. However, higher temperatures may also lead to the formation of toxic transformation products, complicating the treatment outcome. The presence of co-contaminants, including organic matter, metals, and other pollutants, can compete for adsorption sites or react with treatment agents, diminishing the efficiency of PFAS removal processes. Therefore, predictive models must incorporate these environmental variables to simulate realistic PFAS treatment outcomes accurately.

2.4. Bioaccumulation and environmental persistence

PFAS compounds, particularly long-chain variants for instance PFOA and PFOS, are known for their bioaccumulative potential, posing risks to aquatic life and humans (Podder et al., 2021). Due to their stability and resistance to degradation, PFAS can persist in environmental compartments such as groundwater, soil, and sediment for long periods (Zweigle et al., 2023). Bioaccumulation occurs when PFAS compounds enter biological systems and are retained rather than metabolized or excreted. This characteristic increases PFAS concentrations through food webs, posing potential health risks to higher trophic organisms, including humans. The environmental persistence and bioaccumulation of PFAS complicate their remediation, as treatment strategies must not only remove these compounds but also minimize the formation of toxic transformation products that could contribute to ongoing contamination. Predictive models, therefore, need to account for the long-term environmental fate of PFAS, simulating both primary compound removal and the potential risks of any degradation by-products. Fig. 2 depicts the principal health hazards associated with perfluorooctane sulfonate (PFOS) exposure. The diagram classifies these concerns into six principal domains: endocrine disruption, reproductive and developmental toxicity, immune system suppression, carcinogenic risk, cardiovascular and metabolic consequences, and neurotoxicity/liver impairment. The health implications underscore the potential long-term effects of PFOS bioaccumulation and persistence in human populations and ecosystems, highlighting the urgent necessity for additional research and regulatory measures.

2.5. Challenges in modeling PFAS behavior for treatment

The complex interplay of PFAS structure, functional groups, and environmental conditions poses a significant challenge for predictive modeling. Traditional models may not capture the unique properties of each PFAS variant, leading to underestimation or overestimation of treatment efficiency. Developing accurate models requires collecting large and high-quality data, properly reporting data set characteristics, and combining data from multiple institutions with proper normalization on PFAS-specific reaction kinetics, sorption characteristics, and transformation pathways across different treatment scenarios (Yang et al., 2023). Additionally, data scarcity, particularly for emerging PFAS and novel treatment methods, complicates model validation and limits

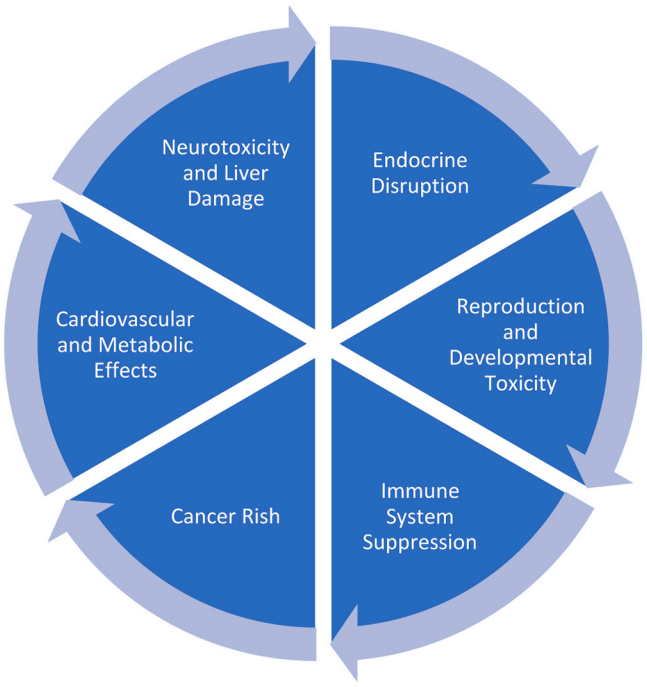

Fig. 2. Health Risks Associated with PFOS Exposure: A Summary.

the applicability of some predictive approaches (Tardioli et al., 2020). Machine learning and data-driven models are beginning to address these challenges by identifying patterns within large datasets using methods like model simplification, optimization approximation, and computation parallelism (Wang et al., 2022); however, interpretability remains an obstacle, as these models may lack the mechanistic insights needed to fully understand PFAS behavior in treatment processes.

3. Overview of predictive modeling approaches for PFAS removal

Predictive modeling for PFAS removal involves the use of computational tools designed to simulate the fate, transport, and degradation pathways of PFAS across various treatment processes (Sima and Jaffé, 2021). These models are invaluable in advancing the understanding of PFAS behavior under different treatment conditions, including reaction kinetics, removal efficiencies, and transformation pathways. Predictive models can be categorized into three main types: empirical models (Gallagher et al., 2021), mechanistic models (Simpson and Maclaren, 2023), and machine learning models (Vora and Iyer, 2018), each with unique strengths and limitations. The choice of model depends on the treatment system's complexity, the specific PFAS compounds targeted, and the availability of relevant data. Table 2 delineates multiple PFAS degrading methods and their efficacy. Electrochemical oxidation and plasma-based technologies provide excellent efficiency and rapid deterioration rates. Advanced reduction techniques exhibit promising outcomes, notably shaped by solution chemistry. Sonolysis and photochemical oxidation exhibit reduced efficacy, with the latter being the least effective technique. Adsorptive photocatalysis is an innovative method characterised by elevated degradation and mineralisation rates. Enzymatic degradation and electroreductive defluorination are nascent approaches with considerable potential, however additional research and optimisation are required.

3.1. Empirical models

Empirical models rely on experimental data to simulate PFAS removal under specific conditions (Xu et al., 2023). These models are often developed from controlled laboratory studies or field data, providing reliable predictions for conditions closely resembling those used in data collection (Njoku, 2017). By incorporating data on observed removal rates, reaction kinetics, and influencing variables, empirical models can offer robust and relatively accurate predictions for similar PFAS and treatment systems. However, their reliance on experimental data limits their generalizability to other settings with differing conditions, treatment methods, or PFAS types. As a result, empirical models are most effective in scenarios where there is a high degree of similarity between the model's training data and the actual treatment conditions, such as in small-scale applications or specific treatment facilities. Recent studies have shown that while empirical models are useful for process-specific applications, their limited adaptability makes them less ideal for large-scale or novel treatment scenarios where variability is high.

Table 2
PFAS degradation techniques and their efficiencies.

Technique	Efficiency	Key Insights
Electrochemical Oxidation	High efficiency, up to 100 % degradation of PFOA under optimal conditions	Effective for both water and wastewater; influenced by current density and treatment time (Uwayezu et al., 2021; Üner et al., 2022).
Advanced Reduction Processes	Promising, highly reductive hydrated electrons (eaq-) enhance degradation	Effective for various PFAS types; influenced by solution chemistry and operating factors (Cui et al., 2020).
Plasma-Based Technology	High efficiency, rapid degradation (e.g., 99 % PFOA in <2.5 min)	Effective for a wide range of pollutants; high energy efficiency; mass-transfer-controlled kinetics (Palma et al., 2021; Saleem et al., 2022).
Sonolysis	High energy demand, less efficient compared to other methods	Noted for high energy consumption; less effective overall (Nzeribe et al., 2019).
Photochemical Oxidation	Ineffective	Least effective method among those reviewed (Nzeribe et al., 2019).
Adsorptive Photocatalysis	> 90 % degradation of PFOA, 62 % mineralization to F-	Combines adsorption and photocatalysis; effective and regenerable material (Li et al., 2020).
Enzymatic Degradation	Potentially effective, still under research	In silico design of enzymes shows promise; future bioengineering needed (Marciesky et al., 2023).
Electroreductive Defluorination	99.81 % removal efficiency, 78.67 % defluorination efficiency	Utilizes quaternary ammonium surfactant-modified cathode; effective at low cathodic potential (Wang et al., 2023).

3.2. Mechanistic models

Mechanistic models simulate PFAS behavior by representing the physical and chemical processes governing PFAS interactions within treatment systems. For instance, this approaches are needed to understand PFAS-soil-water-plant interactions and improve remediation efficiency (Sima and Jaffé, 2021). Unlike empirical models, mechanistic models do not rely solely on experimental data; instead, they incorporate fundamental principles of chemistry and physics to generalize PFAS behavior across different treatment conditions (Reid et al., 2023). For instance, these models account for reaction kinetics, adsorption-desorption processes, and transport dynamics within the treatment medium, making them useful for predicting PFAS removal under a broader range of environmental conditions and treatment types. Mechanistic models can simulate complex treatment processes such as advanced oxidation or electrochemical degradation (Koukkari and

Paiva, 2018), where PFAS removal depends on multiple, interacting factors. Studies on PFAS treatment have demonstrated that mechanistic models are especially valuable for understanding the transformation pathways and potential by-products formed during degradation processes (Clark et al., 2019). However, mechanistic models are data-intensive (Gonçalves et al., 2020), requiring detailed input parameters that may not always be available, especially for newer PFAS compounds or under field conditions with complex water chemistries. Additionally, the computational requirements for mechanistic modeling can be substantial, making them more resource-intensive than empirical approaches (Gherman et al., 2023).

3.3. Machine learning models

Machine learning models represent a data-driven approach to predictive modeling by leveraging on the synthesis of large datasets to identify patterns and relationships in PFAS behavior across treatment processes (Manco et al., 2022). These models use algorithms like ensemble models, artificial neural networks, deep neural networks, recurrent neural networks, and associative reservoir computing to "learn" from data (Bloch, 2023), building predictive functions that can generalize to new, unseen conditions. Machine learning models are particularly advantageous in PFAS modeling as they can analyze extensive data from multiple treatment methods, capturing complex, nonlinear interactions that may be difficult to model mechanistically. For example, machine learning techniques such as neural networks, decision trees, and support vector machines have been employed to predict PFAS removal efficiencies and identify optimal treatment conditions based on input variables like PFAS structure, treatment type, and environmental conditions (Andraju et al., 2023). The scalability and adaptability of machine learning models allow them to offer rapid insights, making them suitable for applications with high variability or limited mechanistic understanding.

Despite their strengths, machine learning models often lack physical interpretability, as they do not inherently provide insights into the underlying mechanisms of PFAS removal (Mi et al., 2020). This limitation makes it challenging to understand the chemical or physical basis of the model's predictions, which may be necessary for applications requiring detailed knowledge of PFAS transformation pathways or by-product formation. Furthermore, machine learning models rely heavily on high-quality, comprehensive datasets, and their predictive accuracy can decline if trained on incomplete or biased data (Andaur Navarro et al., 2021; Miceli et al., 2022; Soni et al., 2023). Current research highlights that while machine learning models are effective for rapid predictions and handling data-intensive scenarios, blending mechanistic and machine-learning approaches can provide similar or better predictive performance and domain interpretability in dynamical systems, with hybrid methods being less data-hungry and more parametrically efficient (Levine and Stuart, 2022).

3.4. Comparative strengths and limitations

Each predictive modeling approach offers distinct benefits depending on the specific requirements and constraints of the treatment scenario. Empirical models are advantageous for their robustness under known conditions but lack generalizability to new settings or PFAS types (Gojić et al., 2023). Mechanistic models provide a deeper understanding of PFAS behavior and transformation within treatment systems, though they are resource-intensive and may be impractical for highly variable conditions. Machine learning models, with their data-driven adaptability and scalability, can handle complex and high-dimensional datasets but often lack the interpretative depth needed to explain the underlying treatment mechanisms.

4. Novel treatment systems for PFAS removal and their modeling needs

The resilience of PFAS compounds against conventional water treatment methods has driven the exploration of novel treatment technologies, including advanced oxidation processes (AOPs), electrochemical systems, nanofiltration, and adsorptive techniques. These technologies offer promising alternatives for effective PFAS removal but are relatively new and often lack extensive, long-term performance data, which complicates the development of predictive models. To effectively simulate PFAS removal and degradation in these novel systems, models must account for factors such as reaction intermediates, the formation of transformation products, and the potential for PFAS reformation under certain treatment conditions. The following sections describe the unique mechanisms, advantages, and modeling requirements of these emerging treatment technologies.

4.1. Advanced oxidation processes (AOPs)

Advanced oxidation processes (AOPs) rely on the generation of highly reactive radicals, such as hydroxyl and sulfate radicals, to degrade PFAS (Xia et al., 2020). Common AOPs include ozonation, photocatalysis, and Fenton reactions, each of which uses specific reactions to generate reactive species that attack PFAS molecules (Malakootian et al., 2020) as depicted in Fig. 3 below. The success of AOPs in PFAS degradation depends on several factors, including the presence of H_2O_2, water matrices, the role of hydroxyl radicals, rate of radical production, the oxidation potential of PFAS, and the pathways through which PFAS molecules transform during treatment (Barisci and Suri, 2021). For instance, studies have shown that PFAS compounds with sulfonate or carboxylate groups degrade at different rates under identical AOP conditions, reflecting the influence of chemical structure on oxidation susceptibility (Zhang et al., 2023).

Predictive modeling for AOPs requires detailed information on radical production rates, which can vary depending on the oxidant, catalyst, and reactor conditions. Additionally, models must simulate the oxidation potential of different PFAS compounds to predict degradation efficiency accurately. Another critical aspect for AOP modeling is the inclusion of transformation pathways, as PFAS compounds often degrade through multiple steps, forming intermediate products before reaching complete mineralization (Singh et al., 2019; Trang et al., 2022). These intermediates may vary in toxicity, so understanding their formation and persistence is essential for accurately assessing the environmental impact of AOP treatment. Therefore, predictive models for AOPs need to integrate these complexities to provide realistic predictions of PFAS degradation under diverse treatment conditions.

4.2. Electrochemical treatment

Electrochemical treatment represents a promising approach for PFAS removal by directly targeting the molecular bonds, particularly the robust carbon-fluorine bonds that characterize these compounds. Electrochemical systems operate by applying a current across electrodes, which generates reactive species capable of degrading PFAS molecules (Radjenovic et al., 2020). This treatment method is advantageous in that it can lead to the breakdown of PFAS into less harmful compounds, and in some cases, complete mineralization as shown in Fig. 3 below. However, the effectiveness of electrochemical treatment depends on variables such as the electrode material, the adsorption behavior of PFAS onto the electrode surface, and the current density applied during treatment.

For predictive modeling of electrochemical degradation, it is crucial to include data on electrode properties, as different electrode materials (e.g., boron-doped diamond, platinum, or graphite) exhibit varying affinities for PFAS and reactive species production rates (Sukeesan et al., 2021). Adsorption behavior is another essential factor, as PFAS

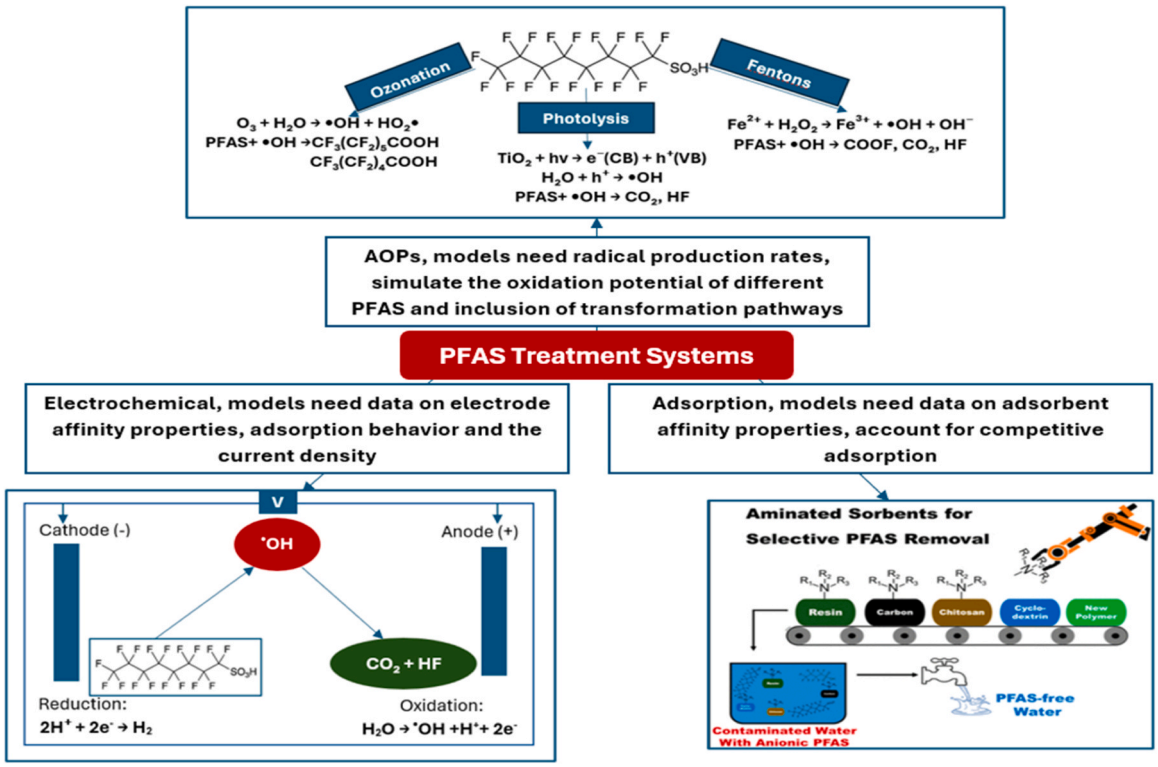

Fig. 3. Illustration summarizing novel treatment technologies for PFAS removal, highlighting mechanisms, and modeling considerations for Advanced Oxidation Processes (AOPs), Electrochemical Treatment, and Adsorptive Techniques.

molecules may interact differently with electrode surfaces based on their specific structures, affecting degradation efficiency. Additionally, current density plays a critical role in generating reactive species and controlling the rate of PFAS breakdown. High current densities may increase degradation rates but also pose the risk of producing unwanted by-products, making it essential for models to balance these dynamics for precise predictions. Predictive models tailored for electrochemical treatment are highly specific to treatment conditions, necessitating site-specific data to optimize PFAS removal and minimize the formation of hazardous transformation products.

4.3. Adsorptive techniques

Adsorptive techniques using materials such as activated carbon and ion-exchange resins are well-established for PFAS removal due to their high capacity to capture contaminants from water. These techniques are primarily based on the physical or chemical attraction of PFAS compounds to the adsorbent surface, removing them from the aqueous phase. Powder activated carbon with higher molecular weight has higher adsorption capacity for long-chain PFAS compounds, achieving 80 % and 90 % equilibria within 60 and 120 minutes, respectively (Son et al., 2020), though short-chain PFAS may require alternative adsorbents such as bio-adsorbents derived from common biomass feedstocks due to their lower affinity for carbon surfaces (Li et al., 2021). Additionally, ion-exchange resins, which operate by exchanging ions between the resin and the water, have also demonstrated promise, especially for shorter-chain PFAS (Dixit et al., 2021).

Predictive modeling for adsorptive techniques must consider the adsorption behavior of different PFAS compounds, as each compound exhibits unique affinity levels based on chain length, functional groups, and ionic characteristics. Additionally, competitive adsorption from co-contaminants present in water can impact PFAS removal efficiency, as other ions or organic molecules may occupy adsorption sites (Wang et al., 2019). Models need to account for this competition to predict when breakthrough, or saturation, might occur, at which point PFAS removal efficiency decreases as shown in Fig. 3 below. Furthermore, certain PFAS compounds may undergo partial desorption under changing environmental conditions, such as pH or temperature fluctuations, which adds complexity to the adsorption process (Kabiri and McLaughlin, 2021). By incorporating these variables, predictive models can estimate the lifespan of adsorptive media and help optimize replacement or regeneration schedules, ensuring continued PFAS removal effectiveness.

5. Integrating PFAS structure and environmental conditions into predictive models

A tailored approach to predictive modeling for PFAS removal is essential due to the structural diversity of PFAS compounds and the significant influence of environmental conditions on their behavior. Incorporating PFAS-specific characteristics, such as chain length and functional groups, alongside environmental factors, such as pH, temperature, isomer structure, and salinity, enables more accurate predictions of PFAS removal in treatment processes (McCleaf et al., 2017). These factors play a critical role in determining PFAS interactions with treatment media, as well as their susceptibility to transformation in processes like oxidation and adsorption. Understanding these variables is essential for building predictive models that can simulate realistic PFAS behavior across diverse treatment scenarios.

5.1. Chain length and functional groups

The chain length of PFAS compounds is a primary structural factor influencing their mobility, bioaccumulation potential, and interaction with treatment systems. Long-chain PFAS, such as PFOA and PFOS, tend to be more hydrophobic and bioaccumulative, often binding more strongly to adsorptive media like activated carbon and ion-exchange resins (Zhang et al., 2019; Zeng et al., 2020). In contrast, short-chain

PFAS compounds exhibit greater mobility in aqueous environments, making them more challenging to capture in adsorption-based treatments and more prone to persistence and spread in water bodies (Li et al., 2020; Román Santiago et al., 2023). Recent studies have highlighted that Short-chain PFAS are more resistant to removal processes that rely on adsorption, necessitating the development of alternative treatment approaches or specialized adsorbents tailored to these smaller molecules such as adding cationic co-surfactant cetrimonium bromide which significantly improves their removal in batch-wise adsorptive bubble separation processes (Stevenson and Karakashev, 2024).

Functional groups attached to the PFAS backbone, such as carboxylate or sulfonate groups, also play a significant role in determining reactivity and treatment efficiency (McCleaf et al., 2017). For example, PFAS compounds with sulfonate groups often demonstrate different adsorption and degradation profiles compared to those with carboxylate groups (Ateia et al., 2019). In oxidative treatment processes, functional groups impact the compound's susceptibility to radical attack, which is essential in advanced oxidation processes. Carboxylate-containing PFAS, for example, may degrade more readily to fluoride ions through a sodium hydroxide-mediated defluorination pathway, potentially offering a new method for PFAS destruction compared to sulfonate-containing PFAS under certain oxidative conditions, a factor that predictive models must incorporate to accurately simulate reaction kinetics and transformation pathways (Trang et al., 2022). Incorporating these structural characteristics into predictive models allows for more precise predictions of treatment outcomes, particularly in systems where PFAS degradation or removal is heavily influenced by molecular structure.

5.2. Environmental factors

Environmental variables, such as pH, temperature, and salinity, which significantly influence PFAS interactions with treatment media and, subsequently, their removal efficiency (Wu et al., 2020; Zhang et al., 2021). pH, for instance, can alter the charge and solubility of PFAS molecules, affecting their adsorption and reactivity in various treatment processes (Wu et al., 2020). At elevated pH levels, some PFAS compounds may undergo deprotonation, leading to a negative charge that can reduce adsorption efficiency on media with similar charges (Wu et al., 2020). Conversely, acidic conditions may enhance PFAS adsorption on certain media, as demonstrated in studies that found increased adsorption efficiency of PFAS onto activated carbon at low pH levels (Zhang et al., 2021). Accurate predictive models for PFAS removal must, therefore, include pH as a variable to simulate realistic interactions between PFAS and treatment media under diverse water chemistry conditions.

Temperature is another crucial environmental factor, impacting reaction rates and sorption behaviors. Higher temperatures generally accelerate reaction kinetics (Bím et al., 2019), potentially improving PFAS degradation in processes such as advanced oxidation or electrochemical treatment. However, elevated temperatures can also lead to the formation of transformation products, which may possess varying degrees of toxicity or persistence. Consequently, predictive models must balance the potential benefits of increased degradation rates with the risks associated with intermediate product formation. In adsorption-based processes, temperature fluctuations can influence the sorption capacity of media, as higher temperatures may reduce adsorption efficiency due to decreased intermolecular forces between PFAS and the adsorbent (Yin et al., 2023).

Salinity, or the concentration of dissolved salts, also affects PFAS removal, particularly in water sources with high ionic content, such as seawater or brackish water, increasing the aggregation and surface activity of PFAS in mixtures, which affect their transport. (Steffens et al., 2023). Salinity can compete with PFAS for adsorption sites on media and, in some cases, disrupt electrostatic interactions essential for PFAS binding. The presence of specific ions, such as sodium and calcium, can compete with PFAS molecules for adsorption sites on media like activated carbon, reducing overall removal efficiency. Including salinity effects in predictive models is particularly important for applications in regions with saltwater intrusion or in specialized applications involving seawater treatment.

5.3. Towards comprehensive and realistic predictive models

Integrating PFAS structure and environmental conditions into predictive models allows for the development of more comprehensive and accurate simulations that reflect the complex interactions governing PFAS removal in treatment processes (Bodner et al., 2020). By accounting for chain length, functional groups, and environmental factors like pH, temperature, and salinity, predictive models can provide more realistic approximations of PFAS behavior in diverse treatment systems. This tailored approach is essential for optimizing treatment strategies, guiding the selection of treatment technologies, and ensuring that models can adapt to the highly variable nature of real-world PFAS contamination scenarios. Ongoing research to refine these models with empirical data on PFAS-specific behavior across different environmental conditions will further enhance their utility, supporting more effective remediation efforts and informed decision-making in PFAS-contaminated environments.

6. Advances in machine learning for PFAS predictive modeling

Machine learning models have become increasingly valuable tools in predictive modeling for PFAS, offering advanced data-driven approaches that enhance the understanding and prediction of PFAS behavior under various treatment conditions. Among these, deep learning models, which use neural networks with multiple layers, are especially effective at capturing complex patterns within large, multidimensional datasets that traditional models may overlook. Machine learning's ability to process and analyze vast volumes of environmental and treatment data allows these models to identify relationships between PFAS characteristics, environmental variables, and treatment efficacy as shown in Fig. 4 below. By recognizing patterns in historical and experimental data, machine learning models can generate predictions for treatment outcomes, often extending to conditions not directly included in the training dataset, making them particularly useful in addressing novel treatment challenges and optimizing remediation strategies for PFAS-contaminated sites.

6.1. Pattern recognition and predictive capabilities

One of the key advantages of machine learning models in PFAS predictive modeling is their ability to handle large and complex datasets, allowing them to extract meaningful patterns across varied treatment scenarios. Machine learning algorithms, including decision trees, support vector machines, and deep neural networks, can be trained on extensive data sources containing information about PFAS structure, environmental conditions, and treatment outcomes (Raza et al., 2019). These algorithms can accurately predict C-F bond dissociation energies in PFAS structures with deviations less than 0.70 kcal/mol (Raza et al., 2019). For instance, machine learning can reveal the complex interactions between PFAS chain length, functional groups, pH, and temperature on adsorption rates in filtration-based systems. Through training on comprehensive datasets, these models become capable of predicting the efficacy of PFAS removal across a wide range of conditions, including scenarios for which empirical or mechanistic data may be limited. This predictive capability is crucial for applications in novel treatment methods, such as advanced oxidation and electrochemical processes, where machine learning models can simulate potential treatment outcomes and optimize conditions for maximum PFAS removal.

Recent studies have demonstrated the predictive strength of machine

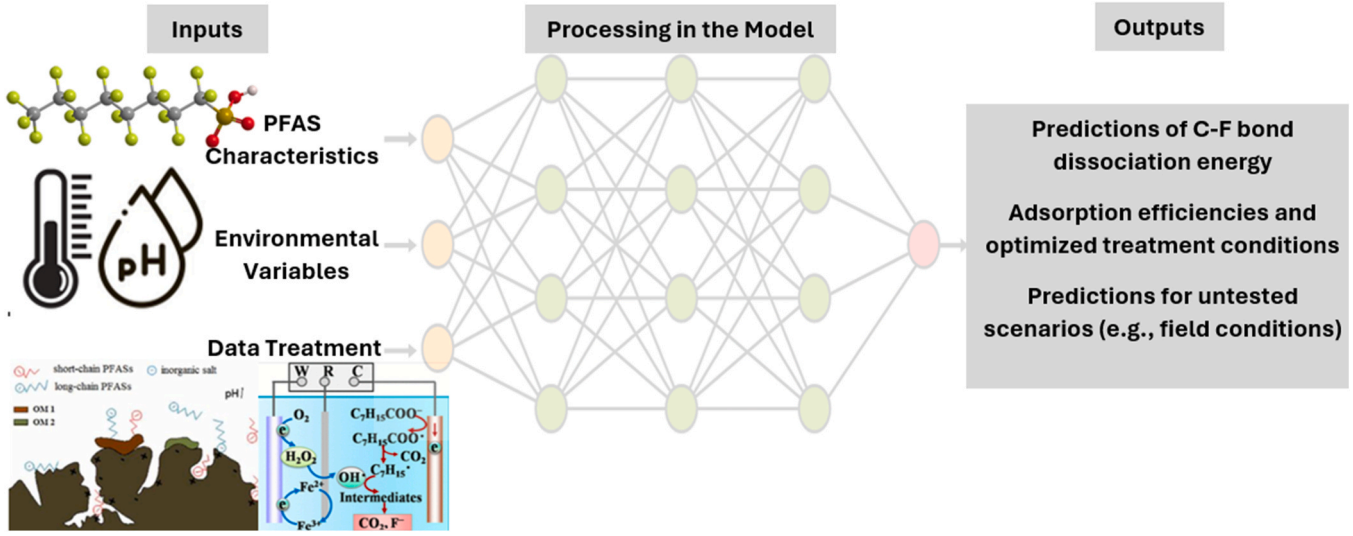

Fig. 4. Integration of Machine Learning for Predictive Modeling in PFAS Treatment: Environmental Inputs, System Processing, and Treatment Outcomes.

learning models for PFAS in applications such as adsorption, degradation, and transport within water matrices. For instance, supervised machine learning models have been trained to predict adsorption efficiencies based on PFAS chain length, media type, and solution chemistry, enabling the identification of the best adsorptive materials for specific PFAS contaminants. Additionally, deep learning models, with their ability to manage high-dimensional data, are increasingly employed to simulate degradation pathways in advanced oxidation processes, providing insights into potential transformation products and the conditions necessary for optimal degradation. By accurately forecasting treatment outcomes, machine learning enhances decision-making for both researchers and regulators, enabling more informed selection and design of treatment systems.

6.2. *Applicability to untested and diverse conditions*

Machine learning models' adaptability makes them particularly well-suited to simulate PFAS treatment outcomes across previously untested or complex environmental conditions. By generalizing patterns from training data, machine learning algorithms can extend predictions to new scenarios, accommodating diverse PFAS compounds, environmental factors, and treatment conditions (Andraju et al., 2023). For example, machine learning models trained on experimental data from laboratory-based PFAS degradation studies can be applied to predict outcomes in field conditions, providing essential information on how treatment performance may vary in real-world applications (Xiao et al., 2023) as depicted in Fig. 4 below. This capability is especially valuable for addressing emerging PFAS compounds for which limited empirical data exists, as well as for adapting treatment models to dynamic conditions, such as seasonal shifts in water chemistry.

Through predictive modeling in untested conditions, machine learning supports the design of adaptable treatment systems that can respond to variability in PFAS contamination profiles and environmental factors. This adaptability also has implications for regulatory planning, as machine learning predictions can offer insight into treatment efficacy under regulatory standards, facilitating compliance with evolving PFAS guidelines. The rapid scalability of machine learning models further enables them to accommodate new data as it becomes available, continuously improving their predictions and supporting more robust treatment designs.

7. Challenges and future directions in PFAS predictive modeling

The development of predictive models for PFAS treatment has brought significant advancements to remediation efforts; however, several challenges remain, limiting the effectiveness and accuracy of these models. Key obstacles include data limitations, issues related to the toxicity of transformation products, and the need for robust model validation (Fàbrega et al., 2014; Feinstein et al., 2021). Addressing these challenges will be essential to enhancing the accuracy and applicability of predictive models in real-world treatment scenarios. Looking forward, future research should prioritize expanding treatment datasets, integrating toxicity assessments, and refining machine learning models for improved interpretability and reliability, ultimately strengthening the role of predictive modeling in PFAS management.

7.1. *Data limitations*

One of the primary challenges in PFAS predictive modeling is the scarcity of comprehensive, long-term treatment data. Many novel PFAS treatment methods, such as advanced oxidation processes and electrochemical systems, are still under development, resulting in limited empirical data on their long-term efficacy and the conditions under which they operate best. In addition, variations in PFAS types, environmental conditions, and treatment system configurations mean that existing data may not be widely generalizable, limiting the predictive power of current models. Without adequate data, predictive models may struggle to accurately simulate PFAS behavior across diverse treatment scenarios, resulting in less reliable outputs for decision-making. Expanding datasets to include long-term performance results across various treatment technologies and PFAS compounds will be crucial for enhancing model accuracy and reliability.

7.2. *Transformation product toxicity*

Predictive models for PFAS treatment often focus primarily on the degradation or removal of parent PFAS compounds but may overlook the formation and potential toxicity of transformation products, which can pose new environmental risks (Raza et al., 2019). During treatment processes such as advanced oxidation or electrochemical degradation, PFAS compounds may undergo partial breakdown, forming intermediate products that retain toxic properties or exhibit persistent behavior (Lotlikar, 2022). These transformation products are not always well-characterized, and their environmental impacts may be unknown, making it difficult for predictive models to simulate the full scope of potential treatment outcomes. Integrating toxicity predictions for transformation products into PFAS models is essential to prevent unintentional environmental or health risks associated with incomplete PFAS

degradation. Achieving this will require toxicological data on PFAS by-products, along with models capable of predicting both the formation of these products and their likely impacts in environmental contexts.

7.3. Model validation

Validation of predictive models through laboratory experiments and field studies is critical for ensuring that models accurately represent PFAS behavior in real-world applications (Dvurecenska et al., 2018). However, many models remain invalidated or partially validated, which raises concerns about their reliability and applicability to field-scale treatment systems. Validation is particularly challenging for machine learning models, which can be highly accurate under training conditions but may fail to generalize when applied to new or varied treatment environments. Current ML data validation methods are difficult to operationalize, yielding too many false positive alerts, requiring manual tuning, or are infeasible at scale (Shankar et al., 2023). To address this, models need to be rigorously tested against empirical data from both lab and field settings, covering a range of PFAS compounds and treatment methods. Model validation should also involve cross-comparison with other models, where possible, to benchmark performance and identify potential areas for improvement. Investing in validation studies will be crucial to establishing predictive models as dependable tools for PFAS treatment planning and regulatory compliance.

7.4. Future directions in PFAS predictive modeling

To overcome these challenges, future research in PFAS predictive modeling should focus on several key areas. Expanding treatment datasets is a priority; as more data is collected from emerging PFAS treatment technologies, models will have a stronger foundation for making accurate predictions. Collaborative data-sharing efforts among researchers, industries, and regulatory bodies could facilitate the rapid expansion of these datasets, capturing a wide range of PFAS behaviors under diverse environmental and treatment conditions. Additionally, incorporating toxicity predictions for transformation products is essential to address the risks associated with incomplete PFAS degradation. By integrating toxicological data on PFAS by-products and assessing their persistence and mobility, predictive models can provide a more comprehensive evaluation of treatment outcomes.

Further refining machine learning models will also play a crucial role in future advancements. While machine learning has proven valuable for pattern recognition and prediction, enhancing interpretability and transparency will be essential to increasing their utility and trustworthiness in environmental applications. Techniques such as explainable artificial intelligence (XAI) and hybrid modeling approaches that combine mechanistic insights with data-driven methods can improve the interpretability of machine learning models, making them more accessible and informative for researchers and decision-makers. Transfer learning, a method that enables models trained on one dataset to be applied to similar but distinct datasets, may also offer a solution to data limitations by allowing for greater generalizability across diverse PFAS compounds and treatment types.

8. Conclusion

Predictive modeling has emerged as an essential tool in evaluating and enhancing PFAS removal and degradation in advanced treatment systems. By incorporating PFAS-specific characteristics, such as chain length and functional groups, along with key environmental factors and treatment types, these models enable the development of targeted remediation strategies that can address the unique challenges posed by PFAS contamination. Through detailed simulations, predictive models provide valuable insights into degradation pathways, reaction kinetics, and treatment efficiencies, supporting decision-making processes aimed at optimizing treatment approaches and reducing environmental impact.

Looking to the future, advancements in data collection, model complexity, and the integration of machine learning will likely improve the accuracy and applicability of these predictive tools. Expanded datasets from field and laboratory studies, covering a range of PFAS compounds and novel treatment conditions, will enhance model accuracy and generalizability. Additionally, integrating machine learning techniques and developing hybrid models that combine mechanistic and data-driven approaches hold promise for capturing complex PFAS behaviors while improving model interpretability. These advancements will empower decision-makers with the tools and insights needed to address PFAS contamination in a more sustainable, effective manner, ultimately contributing to safer water resources and a healthier environment.

CRediT authorship contribution statement

Olawade David: Conceptualization, Investigation, Methodology, Project administration, Writing – original draft, Writing – review & editing. **Olajoyetan David:** Investigation, Validation, Writing – original draft, Writing – review & editing. **Wada Ojima:** Investigation, Methodology, Supervision, Writing – original draft, Writing – review & editing. **Ige Abimbola:** Visualization, Writing – original draft, Writing – review & editing. **Ijiwade James:** Data curation, Formal analysis, Investigation, Methodology, Visualization, Writing – original draft, Writing – review & editing. **Fapohunda Oluwaseun:** Investigation, Methodology, Writing – original draft, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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